CALCULATION OF THERMODYNAMIC PARAMETERS OF DERIVATIVES OF POLYCHLORINATED BIPHENYLS

A.V. Maiorova [1*], T.V. Kulikova [1], K.Yu. Shunyaev [1]

[1] Institute of Metallurgy of the Ural Branch, Russian Academy of Sciences, 101 Amundsena st., Yekaterinburg, 620016, Russia

** e-mail: imeturoran@mail.ru*

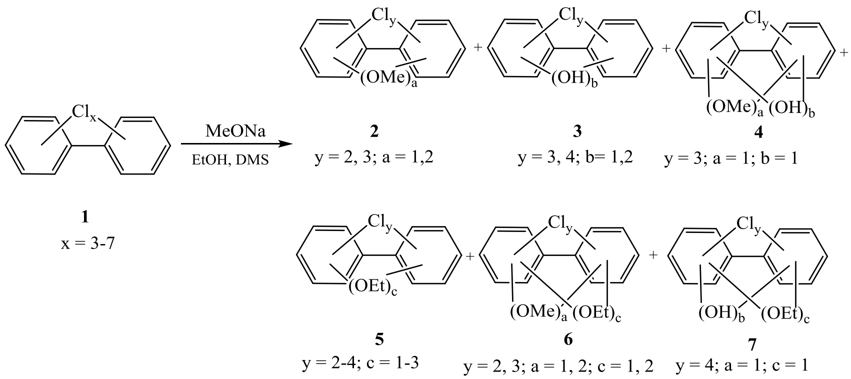
Thermochemical parameters, such as standard enthalpy of formation, enthalpy increment from 0 to 298 K, standard heat capacity and its temperature dependence, and entropy, were calculated for the ethoxy-, ethoxymethoxy- and ethoxyhydroxy- derivatives formed from polychlorinated biphenyls congeners by chemical interaction with sodium methoxide in dimethyl sulfoxide and ethanol.

Introduction

Polychlorinated biphenyls (PCBs) are the most ubiquitous anthropogenic pollutants. The Stockholm Convention (2001) requires PCBs to be completely destroyed by 2025. According to different sources, from 180 to 500 tons of PCB of different trademarks were produced in Russia over the period from 1939 to 1990 [1, 2]. At present no technology capable of destroying all PCB stocks is available. The only way to utilize these toxic wastes is to combine several processing technologies [3, 4]. Promising technologies for detoxification of PCBs or their pretreatment for the subsequent destruction are based on chemical reactions of PCBs. The most widespread of such technologies involves nucleophilic substitution of aromatically bound chlorine atoms in PCBs by other substituents, for example, alkoxy groups [4]. The procedures of PCB alkoxylation are simple to realize and do not require special equipment. However, in view of the fact that any commercial PCB trademark is a mixture of several tens of congeners, and the behavior of each congener in one or another chemical reaction is hardly predictable. One of the first PCB alkoxylation processes thoroughly studied by gas chromatography–mass spectrometry is the reaction of the technical mixture Sovol by sodium methoxide (MeONa) in dimethyl sulfoxide (DMS) and methanol (MeOH) [4, 5].

Thermodynamic modeling (TDM) aimed at finding conditions ensuring the formation of the maximal amount of hydrophilic PCB in nucleophilic substitution reactions is a topical problem. The use of TDM allows significant saving of materials, labor, and time and reduces to a minimum the contact of researchers with toxic substances. TDM allows finding complete equilibrium chemical composition of the system at the preset thermodynamic parameters (e.g., temperature and pressure). HSC program for calculating the multicomponent high-temperature equilibrium is used for these purposes [6]. The TDM method was successfully used previously for calculating the composition of products formed by chemical and thermal reprocessing of toxic PCBs [4, 7, 8]. Thermodynamic modeling has not been applied to the reaction of the technical mixture Sovol by MeONa in DMS and ethanol EtOH (SCHEME).

SCHEME



The necessary condition for the realization of the TDM of our research is the availability of a database of thermochemical parameters of the compounds of interest. The following thermochemical parameters are required for thermodynamic modeling of derivatives of PCBs: standard enthalpy of formation (ΔH^0_{298}), enthalpy increment from 0 to 298 K ($H^0_{298} - H^0_0$), standard heat capacity ($C_p{}^0_{298}$) and its temperature dependence [$C_p(T)$], entropy (S^0_{298}), etc. These data are scarcely available in the literature. The thermochemical properties of the methoxy- **2**, hydroxyl- **3** and methoxyhydroxy- **4** derivatives have been calculated and reported by us earlier [7, 9]. The data on derivatives ethoxy- **5**, ethoxymethoxy- **6,** ethoxyhydroxy- **7** PCBs have not been available.

This study aimed to calculated thermochemical parameters for the ethoxy- **5**, ethoxymethoxy- **6** ethoxyhydroxy- **7** derivatives formed from polychlorinated biphenyls congeners by chemical interaction with sodium methoxide in dimethyl sulfoxide and ethanol.

Results and discussion

Calculation of thermodynamic parameters of ethoxy-, ethoxymethoxy-, ethoxyhydroxy- derivatives of polychlorinated biphenyls

The standard enthalpy of formation, Gibbs energies, and heat capacity of **5, 6, 7** derivatives were calculated using the ChemBioDraw Ultra 12.0. software and Jobak method [10], which are based on an analysis of the molecular structure. As concrete derivatives we chose compounds derived from those PCBs congeners which are really present in Sovol (Table 1).

The standard entropy was calculated by Eq. (1).

$$\Delta S^0_{298} = (\Delta H^0_{298} - \Delta G^0_{298})/298.15. \tag{1}$$

The standard enthalpies of formation and Gibbs energies used in Eq. (1) were calculated by the ChemBioDraw Ultra 12.0 software, and the standard entropies of the starting compounds were calculated by Eqs. (2) and (3) using the reference data in [11].

$$\Delta S^0_{298} = S^0_{298\ \text{product}} - \Sigma S^0_{298\ \text{start.comp.}}, \tag{2}$$

$$S^0_{298\ \text{product}} = \Sigma S^0_{298\ \text{start.comp}}. + (\Delta H^0_{298} - \Delta G^0_{298})/298.15. \tag{3}$$

The temperature dependence heat capacity of 5, 6, 7 derivatives were calculated using Jobak method calculations [10]. The resulting data were fitted by the polynomial (4).

$$C_p\,(T) = a + b\times10^{-3}T + c\times10^{5}T^{-2} + d\times10^{-6}T^{2}. \tag{4}$$

Table 1

PCBs derivatives used for modeling the chemical reaction with sodium methoxide

№	Starting congener (content in Sovol, %)	positions of derivatives / chlorine atoms
1	PCB 28 (0.4)	2- / 4,4'- 2,4- / 4'- 2,4,4'- / -
2	PCB 47 (0.5)	2- / 2',4,4'- 2,2'- / 4,4'- 2,2',4- / 4'- 2,2',4,4'- / -
3	PCB 118 (11.1)	4'- / 2,4,5,3'- 5,4'- / 2,4,3'- 4,5,4'- / 2,3'- 4,5,3',4'- / 2- 2,4,5,3',4'- / -
4	PCB 153 (6.1)	5'- / 2,4,5,2',4'- 5,5'- / 2,4,2',4'- 5,4',5'- / 2,4,2'- 5,2',4',5'- / 2,4- 4,5,2',4',5'- / 2- 2,4,5,2',4',5'- / -
5	PCB 180 (0.6)	4- / 2,3,5,2',4',5'- 4,5'- / 2,3,5,2',4'- 4,5,5'- / 2,3,2',4'- 4,5,2',5'- / 2,3,4'- 4,5,2',4',5'- / 2,3- 2,4,5,2',4',5'- / 3- 2,3,4,5,2',4',5'- / -

The enthalpy increment from 0 to 298 K was calculated by Eq. (5) [12].

$$H^{0}_{298} - H^{o}_{0} \approx 0.5 C_{p}{}^{o}{}_{298} \cdot 298.15. \qquad (5)$$

The calculated values of all the above-mentioned thermochemical parameters of the ethoxy- **5**, ethoxymethoxy- **6,** ethoxyhydroxy- **7** derivatives PCBs are listed in Table 2 and thermodynamic modeling here been applied to the reaction of the technical mixture Sovol by MeONa in DMS and ethanol EtOH (SCHEME).

Table 2

Thermochemical parameters of derivatives **5, 6, 7** PCBs

Compound	ΔH^o_{298}, kJ mol^{-1}	S^o_{298}, J mol^{-1} K^{-1}	ΔG^o_{298}, kJ mol^{-1}	H^o_{298}-H^o_o, kJ mol^{-1}
$C_{12}H_7Cl_2(OC_2H_5)$	-57.34	542.46	134.07	37.95
$C_{12}H_7Cl(OC_2H_5)_2$	-215.1	597.41	57.84	45.03
$C_{12}H_7(OC_2H_5)_3$	-372.86	652.36	-18.39	52.11
$C_{12}H_6Cl_3(OC_2H_5)$	-84.55	569.60	112.51	40.21
$C_{12}H_6Cl_2(OC_2H_5)_2$	-242.31	624.55	36.28	47.30
$C_{12}H_6Cl(OC_2H_5)_3$	-400.07	679.50	-39.95	54.38
$C_{12}H_6(OC_2H_5)_4$	-557.83	734.45	-116.18	61.46
$C_{12}H_5Cl_4(OC_2H_5)$	-111.76	596.75	90.95	42.48
$C_{12}H_5Cl_3(OC_2H_5)_2$	-269.52	651.69	14.72	49.56
$C_{12}H_5Cl_2(OC_2H_5)_3$	-427.28	706.64	-61.51	56.64
$C_{12}H_5Cl(OC_2H_5)_4$	-585.04	761.59	-137.74	63.72
$C_{12}H_5(OC_2H_5)_5$	-742.80	816.54	-213.97	70.80
$C_{12}H_4Cl_5(OC_2H_5)$	-138.97	623.89	69.39	44.75
$C_{12}H_4Cl_4(OC_2H_5)_2$	-296.73	678.83	-6.84	51.83
$C_{12}H_4Cl_3(OC_2H_5)_3$	-454.49	733.78	-83.07	58.91
$C_{12}H_4Cl_2(OC_2H_5)_4$	-612.25	788.73	-159.30	65.99
$C_{12}H_4Cl(OC_2H_5)_5$	-770.01	843.68	-235.53	73.07
$C_{12}H_4(OC_2H_5)_6$	-927.77	898.63	-311.76	80.15
$C_{12}H_3Cl_6(OC_2H_5)$	-166.18	651.03	47.83	47.01
$C_{12}H_3Cl_5(OC_2H_5)_2$	-323.94	705.98	-28.40	54.09
$C_{12}H_3Cl_4(OC_2H_5)_3$	-481.70	760.92	-104.63	61.17
$C_{12}H_3Cl_3(OC_2H_5)_4$	-639.46	815.87	-180.86	68.26
$C_{12}H_3Cl_2(OC_2H_5)_5$	-797.22	870.82	-257.09	75.34
$C_{12}H_3Cl(OC_2H_5)_6$	-954.98	925.77	-333.32	82.42
$C_{12}H_3(OC_2H_5)_7$	-1112.74	980.72	-409.55	89.50
$C_{12}H_6Cl_2(OC_2H_5)OCH_3$	-221.67	586.00	27.86	43.89
$C_{12}H_5Cl_3(OC_2H_5)OCH_3$	-248.88	613.14	6.30	46.16
$C_{12}H_5Cl_2(OC_2H_5)_2OCH_3$	-406.64	668.09	-69.93	53.26
$C_{12}H_4Cl_4(OC_2H_5)OCH_3$	-276.09	640.28	-15.26	48.43
$C_{12}H_4Cl_3(OC_2H_5)_2OCH_3$	-433.85	695.23	-91.49	55.54

Compound	ΔH^o_{298}, kJ mol^{-1}	S^o_{298}, J mol^{-1} K^{-1}	ΔG^o_{298}, kJ mol^{-1}	H^o_{298}-H^o_o, kJ mol^{-1}
$C_{12}H_4Cl_3(OC_2H_5)(OCH_3)_2$	-413.21	656.68	-99.91	52.10
$C_{12}H_3Cl_4(OC_2H_5)(OCH_3)_2$	-440.42	683.82	-121.47	54.37
$C_{12}H_5Cl_2(OC_2H_5)(OCH_3)_2$	-386	629.54	-78.35	49.83
$C_{12}H_6Cl(OC_2H_5)(OCH_3)_2$	-358.79	602.40	-56.79	47.54
$C_{12}H_6(OC_2H_5)(OCH_3)_3$	-495.91	618.80	-141.44	51.23
$C_{12}H_6(OC_2H_5)_2(OCH_3)_2$	-516.55	657.35	-133.02	54.64
$C_{12}H_6(OC_2H_5)_3(OCH_3)$	-537.19	695.89	-124.60	58.09
$C_{12}H_5Cl(OC_2H_5)(OCH_3)_3$	-523.12	645.94	-163.00	53.50
$C_{12}H_5(OC_2H_5)(OCH_3)_4$	-660.24	662.34	-247.65	57.17
$C_{12}H_5(OC_2H_5)_2(OCH_3)_3$	-680.88	700.88	-239.23	60.60
$C_{12}H_5(OC_2H_5)_3(OCH_3)_2$	-701.52	739.43	-230.81	64.03
$C_{12}H_5(OC_2H_5)_4(OCH_3)$	-722.16	2204.33	-222.39	57.18
$C_{12}H_4Cl_2(OC_2H_5)(OCH_3)_3$	-550.33	673.08	-184.56	55.77
$C_{12}H_4Cl(OC_2H_5)(OCH_3)_4$	-687.45	689.48	-269.21	59.44
$C_{12}H_4(OC_2H_5)(OCH_3)_5$	-824.37	706.56	-353.86	63.11
$C_{12}H_4(OC_2H_5)_2(OCH_3)_4$	-845.21	744.42	-345.44	66.54
$C_{12}H_4(OC_2H_5)_3(OCH_3)_3$	-865.85	783.04	-337.04	69.97
$C_{12}H_4(OC_2H_5)_4(OCH_3)_2$	-886.49	821.52	-328.60	73.40
$C_{12}H_4(OC_2H_5)_5(OCH_3)$	-907.13	860.07	-320.18	76.84
$C_{12}H_4Cl_2(OC_2H_5)_2(OCH_3)_2$	-570.97	711.96	-176.24	59.20
$C_{12}H_4Cl_2(OC_2H_5)_3(OCH_3)$	-591.61	665.57	-167.72	62.64
$C_{12}H_4Cl(OC_2H_5)_2(OCH_3)_3$	-708.09	728.02	-260.79	62.87
$C_{12}H_4Cl(OC_2H_5)_3(OCH_3)_2$	-728.73	766.57	-252.37	66.30
$C_{12}H_4Cl(OC_2H_5)_4(OCH_3)$	-749.37	805.12	-243.95	69.74
$C_{12}H_5Cl(OC_2H_5)_2(OCH_3)_2$	-543.76	684.49	-154.58	56.93
$C_{12}H_5Cl(OC_2H_5)_3(OCH_3)$	-564.4	723.03	-146.16	60.37
$C_{12}H_3Cl_4(OC_2H_5)_2(OCH_3)$	-448.08	603.47	-64.64	61.07
$C_{12}H_3C_{l3}(OC_2H_5)_3(OCH_3)$	-618.82	777.31	-189.28	64.91
$C_{12}H_3Cl_3(OC_2H_5)_2(OCH_3)_2$	-598.18	738.77	-197.70	61.47
$C_{12}H_3Cl_3(OC_2H_5)(OCH_3)_3$	-577.54	700.22	-206.12	58.04
$C_{12}H_3Cl_2(OC_2H_5)_2(OCH_3)_3$	-735.3	754.59	-282.18	65.14
$C_{12}H_3Cl_2(OC_2H_5)_3(OCH_3)_2$	-755.94	793.71	-273.93	68.57
$C_{12}H_3Cl_2(OC_2H_5)_4(OCH_3)$	-776.58	832.26	-290.77	72.01
$C_{12}H_3Cl_2(OC_2H_5)(OCH_3)_4$	-714.66	716.62	-290.77	61.71
$C_{12}H_3Cl(OC_2H_5)(OCH_3)_5$	-851.78	733.03	-375.42	65.38
$C_{12}H_3Cl(OC_2H_5)_5(OCH_3)_1$	-934.34	887.21	-341.74	79.11
$C_{12}H_3Cl(OC_2H_5)_4(OCH_3)_2$	-913.7	848.66	-350.16	76.71

Compound	ΔH^o_{298}, kJ mol^{-1}	S^o_{298}, J mol^{-1} K^{-1}	ΔG^o_{298}, kJ mol^{-1}	H^o_{298}-H^o_o, kJ mol^{-1}
$C_{12}H_3Cl(OC_2H_5)_3(OCH_3)_3$	-893.05	810.14	-358.58	72.13
$C_{12}H_3Cl(OC_2H_5)_2(OCH_3)_4$	-872.42	771.56	-367.00	68.67
$C_{12}H_3(OC_2H_5)_2(OCH_3)_5$	-1009.54	787.97	-451.65	72.48
$C_{12}H_3(OC_2H_5)(OCH_3)_6$	-988.9	749.43	-460.07	69.05
$C_{12}H_3(OC_2H_5)_6(OCH_3)$	-1092.1	942.15	-417.97	86.21
$C_{12}H_3(OC_2H_5)_5(OCH_3)_2$	-1071.46	903.60	-426.39	82.77
$C_{12}H_3(OC_2H_5)_4(OCH_3)_3$	-1050.82	865.06	-434.81	79.35
$C_{12}H_3(OC_2H_5)_3(OCH_3)_4$	-1030.18	826.51	-443.23	75.91
$C_{12}H_6Cl_2(OC_2H_5)OH$	-234.65	568.82	-20.55	40.62
$C_{12}H_5Cl_3(OC_2H_5)OH$	-261.86	595.96	-42.11	42.89
$C_{12}H_5Cl_2(OC_2H_5)_2OH$	-419.62	650.91	-118.34	49.99
$C_{12}H_4Cl_4(OC_2H_5)OH$	-289.07	623.10	-63.67	45.16
$C_{12}H_4Cl_3(OC_2H_5)_2OH$	-446.83	678.05	-139.90	52.27
$C_{12}H_4Cl_3(OC_2H_5)(OH)_2$	-439.17	622.32	-196.73	45.57
$C_{12}H_3Cl_4(OC_2H_5)(OH)_2$	-466.38	649.46	-218.29	47.84
$C_{12}H_5Cl_2(OC_2H_5)(OH)_2$	-411.96	595.18	-175.17	43.30
$C_{12}H_6Cl(OC_2H_5)(OH)_2$	-384.75	568.04	-153.61	41.01
$C_{12}H_6(OC_2H_5)(OH)_3$	-534.85	567.26	-286.67	41.43
$C_{12}H_6(OC_2H_5)_2(OH)_2$	-542.51	622.99	-229.84	48.11
$C_{12}H_6(OC_2H_5)_3(OH)$	-550.17	678.71	-173.01	54.82
$C_{12}H_5Cl(OC_2H_5)(OH)_3$	-562.06	594.40	-308.23	43.70
$C_{12}H_5(OC_2H_5)(OH)_4$	-712.16	593.62	-441.29	44.11
$C_{12}H_5(OC_2H_5)_2(OH)_3$	-719.82	649.34	-384.46	50.80
$C_{12}H_5(OC_2H_5)_3(OH)_2$	-727.48	705.07	-327.63	57.50
$C_{12}H_5(OC_2H_5)_4(OH)$	-735.14	2187.15	-270.80	53.91
$C_{12}H_4Cl_2(OC_2H_5)(OH)_3$	-589.27	621.54	-329.79	45.97
$C_{12}H_4Cl(OC_2H_5)(OH)_4$	-739.37	620.76	-462.85	46.38
$C_{12}H_4(OC_2H_5)(OH)_5$	-889.27	620.65	-595.91	46.78
$C_{12}H_4(OC_2H_5)_2(OH)_4$	-897.13	675.70	-539.08	53.48
$C_{12}H_4(OC_2H_5)_3(OH)_3$	-904.79	731.50	-482.27	60.17
$C_{12}H_4(OC_2H_5)_4(OH)_2$	-912.45	787.16	-425.42	66.87
$C_{12}H_4(OC_2H_5)_5(OH)$	-920.11	842.89	-368.59	73.57
$C_{12}H_4Cl_2(OC_2H_5)_2(OH)_2$	-596.93	677.60	-273.06	52.67
$C_{12}H_4Cl_2(OC_2H_5)_3(OH)$	-604.59	648.39	-216.13	59.37
$C_{12}H_4Cl(OC_2H_5)_2(OH)_3$	-747.03	676.48	-406.02	53.07
$C_{12}H_4Cl(OC_2H_5)_3(OH)_2$	-754.69	732.21	-349.19	59.77
$C_{12}H_4Cl(OC_2H_5)_4(OH)$	-762.35	787.94	-292.36	66.47

Compound	ΔH^o_{298}, kJ mol^{-1}	S^o_{298}, J mol^{-1} K^{-1}	ΔG^o_{298}, kJ mol^{-1}	H^o_{298}-H^o_o, kJ mol^{-1}
$C_{12}H_5Cl(OC_2H_5)_2(OH)_2$	-569.72	650.13	-251.40	50.40
$C_{12}H_5Cl(OC_2H_5)_3(OH)$	-577.38	705.85	-194.57	57.10
$C_{12}H_3Cl_4(OC_2H_5)_2(OH)$	-461.06	586.29	-113.05	57.80
$C_{12}H_3Cl_3(OC_2H_5)_3(OH)$	-631.8	760.13	-237.69	61.64
$C_{12}H_3Cl_3(OC_2H_5)_2(OH)_2$	-624.14	704.41	-294.52	54.94
$C_{12}H_3Cl_3(OC_2H_5)(OH)_3$	-616.48	648.68	-351.35	48.24
$C_{12}H_3Cl_2(OC_2H_5)_2(OH)_3$	-774.24	703.05	-427.41	55.34
$C_{12}H_3Cl_2(OC_2H_5)_3(OH)_2$	-781.9	759.35	-370.75	62.04
$C_{12}H_3Cl_2(OC_2H_5)_4(OH)$	-789.56	815.08	-339.18	68.74
$C_{12}H_3Cl_2(OC_2H_5)(OH)_4$	-766.58	647.90	-484.41	48.65
$C_{12}H_3Cl(OC_2H_5)(OH)_5$	-916.68	647.12	-617.47	49.05
$C_{12}H_3Cl(OC_2H_5)_5(OH)$	-947.32	870.03	-390.15	75.84
$C_{12}H_3Cl(OC_2H_5)_4(OH)_2$	-939.66	814.30	-446.98	70.18
$C_{12}H_3Cl(OC_2H_5)_3(OH)_3$	-931.99	758.60	-503.81	62.33
$C_{12}H_3Cl(OC_2H_5)_2(OH)_4$	-924.34	702.84	-560.64	55.61
$C_{12}H_3(OC_2H_5)_2(OH)_5$	-1074.44	702.06	-693.70	56.15
$C_{12}H_3(OC_2H_5)(OH)_6$	-1066.78	646.34	-750.53	49.46
$C_{12}H_3(OC_2H_5)_6(OH)$	-1105.08	924.97	-466.38	82.94
$C_{12}H_3(OC_2H_5)_5(OH)_2$	-1097.42	869.24	-523.21	76.24
$C_{12}H_3(OC_2H_5)_4(OH)_3$	-1089.76	813.52	-580.04	69.55
$C_{12}H_3(OC_2H_5)_3(OH)_4$	-1082.1	757.79	-636.87	62.85

Table 2 (continued)

Compound	$C_p = a + b\cdot10^{-3} T + c\cdot10^{5} T^{-2} + d\cdot10^{-6} T^{2}$ J mol^{-1} K^{-1}			
	a	b	c	d
$C_{12}H_7Cl_2(OC_2H_5)$	48.617	817.79	-6.88	-338.97
$C_{12}H_7Cl(OC_2H_5)_2$	45.884	992.63	-3.98	-396.42
$C_{12}H_7(OC_2H_5)_3$	43.151	1167.47	-1.08	-453.86
$C_{12}H_6Cl_3(OC_2H_5)$	70.43	786.89	-5.73	-324.15
$C_{12}H_6Cl_2(OC_2H_5)_2$	67.69	961.73	-2.83	-381.59
$C_{12}H_6Cl(OC_2H_5)_3$	64.97	1136.57	0.07	-439.04
$C_{12}H_6(OC_2H_5)_4$	62.23	1311.41	2.97	-496.49
$C_{12}H_5Cl_4(OC_2H_5)$	92.24	755.99	-4.57	-309.33
$C_{12}H_5Cl_3(OC_2H_5)_2$	89.51	930.83	-1.67	-366.77
$C_{12}H_5Cl_2(OC_2H_5)_3$	86.78	1105.67	1.22	-424.22
$C_{12}H_5Cl(OC_2H_5)_4$	84.05	1280.51	4.12	-481.67

Compound	$C_p = a + b \cdot 10^{-3} T + c \cdot 10^5 T^{-2} + d \cdot 10^{-6} T^2$ J mol^{-1} K^{-1}			
	a	b	c	d
$C_{12}H_5(OC_2H_5)_5$	81.31	1455.35	7.02	-539.11
$C_{12}H_4Cl_5(OC_2H_5)$	114.06	725.09	-3.42	-294.51
$C_{12}H_4Cl_4(OC_2H_5)_2$	111.32	899.93	-0.52	-351.95
$C_{12}H_4Cl_3(OC_2H_5)_3$	108.59	1074.77	2.38	-409.39
$C_{12}H_4Cl_2(OC_2H_5)_4$	105.86	1249.61	5.27	-466.85
$C_{12}H_4Cl(OC_2H_5)_5$	103.13	1424.45	8.17	-524.29
$C_{12}H_4(OC_2H_5)_6$	100.39	1599.29	11.07	-581.74
$C_{12}H_3Cl_6(OC_2H_5)$	135.87	694.19	-2.27	-279.68
$C_{12}H_3Cl_5(OC_2H_5)_2$	133.14	869.03	0.63	-337.13
$C_{12}H_3Cl_4(OC_2H_5)_3$	130.41	1043.87	3.53	-394.58
$C_{12}H_3Cl_3(OC_2H_5)_4$	127.67	1218.71	6.43	-452.02
$C_{12}H_3Cl_2(OC_2H_5)_5$	124.94	1393.55	9.32	-509.47
$C_{12}H_3Cl(OC_2H_5)_6$	122.21	1568.39	12.22	-566.92
$C_{12}H_3(OC_2H_5)_7$	119.48	1743.23	15.12	-624.36
$C_{12}H_6Cl_2(OC_2H_5)OCH_3$	64.58	883.05	-1.96	-351.01
$C_{12}H_5Cl_3(OC_2H_5)OCH_3$	83.66	859.70	0.09	-341.54
$C_{12}H_5Cl_2(OC_2H_5)_2OCH_3$	81.91	1067.43	-0.94	-435.70
$C_{12}H_4Cl_4(OC_2H_5)OCH_3$	102.74	836.34	2.15	-332.06
$C_{12}H_4Cl_3(OC_2H_5)_2OCH_3$	117.11	985.86	-2.97	-352.36
$C_{12}H_4Cl_3(OC_2H_5)(OCH_3)_2$	75.43	955.00	16.60	-362.17
$C_{12}H_3Cl_4(OC_2H_5)(OCH_3)_2$	94.51	931.54	18.65	-352.75
$C_{12}H_5Cl_2(OC_2H_5)(OCH_3)_2$	56.35	978.46	14.54	-371.70
$C_{12}H_6Cl(OC_2H_5)(OCH_3)_2$	37.28	1001.92	12.49	-381.17
$C_{12}H_6(OC_2H_5)(OCH_3)_3$	9.97	1120.78	26.94	-411.34
$C_{12}H_6(OC_2H_5)_2(OCH_3)_2$	45.27	1174.63	8.99	-430.69
$C_{12}H_6(OC_2H_5)_3(OCH_3)$	97.71	1166.79	2.17	-371.51
$C_{12}H_5Cl(OC_2H_5)(OCH_3)_3$	29.05	1097.32	29.00	-401.87
$C_{12}H_5(OC_2H_5)(OCH_3)_4$	1.74	1216.18	43.45	-432.03
$C_{12}H_5(OC_2H_5)_2(OCH_3)_3$	35.10	1277.01	25.99	-460.27
$C_{12}H_5(OC_2H_5)_3(OCH_3)_2$	104.89	1206.65	-0.70	-321.61
$C_{12}H_5(OC_2H_5)_4(OCH_3)$	124.48	1317.14	-14.67	-412.96
$C_{12}H_4Cl_2(OC_2H_5)(OCH_3)_3$	48.12	1073.86	31.05	-392.39
$C_{12}H_4Cl(OC_2H_5)(OCH_3)_4$	20.82	1192.72	45.50	-422.56
$C_{12}H_4(OC_2H_5)(OCH_3)_5$	-6.49	1311.58	59.95	-452.72
$C_{12}H_4(OC_2H_5)_2(OCH_3)_4$	19.07	1400.55	44.47	-516.72
$C_{12}H_4(OC_2H_5)_3(OCH_3)_3$	44.62	1489.62	28.99	-580.72
$C_{12}H_4(OC_2H_5)_4(OCH_3)_2$	70.18	1578.60	13.51	-644.73
$C_{12}H_4(OC_2H_5)_5(OCH_3)$	95.73	1667.57	-1.97	-1037.77

Compound	$C_p = a + b\cdot10^{-3}\,T + c\cdot10^{5}\,T^{-2} + d\cdot10^{-6}\,T^{2}$ J mol^{-1} K^{-1}			
	a	b	c	d
$C_{12}H_4Cl_2(OC_2H_5)_2(OCH_3)_2$	73.68	1162.83	15.57	-456.39
$C_{12}H_4Cl_2(OC_2H_5)_3(OCH_3)$	99.24	1251.90	0.09	-520.39
$C_{12}H_4Cl(OC_2H_5)_2(OCH_3)_3$	46.37	1281.69	30.02	-486.56
$C_{12}H_4Cl(OC_2H_5)_3(OCH_3)_2$	89.89	1306.03	9.99	-468.28
$C_{12}H_4Cl(OC_2H_5)_4(OCH_3)$	97.48	1459.74	-0.94	-614.56
$C_{12}H_5Cl(OC_2H_5)_2(OCH_3)_2$	54.60	1186.29	13.51	-465.87
$C_{12}H_5Cl(OC_2H_5)_3(OCH_3)$	80.16	1275.36	-1.97	-529.87
$C_{12}H_3Cl_4(OC_2H_5)_2(OCH_3)$	120.07	1020.51	3.17	-416.75
$C_{12}H_3C_{l3}(OC_2H_5)_3(OCH_3)$	118.31	1228.44	2.14	-510.92
$C_{12}H_3Cl_3(OC_2H_5)_2(OCH_3)_2$	92.76	1139.37	17.62	-446.92
$C_{12}H_3Cl_3(OC_2H_5)(OCH_3)_3$	44.96	1130.57	38.74	-484.83
$C_{12}H_3Cl_2(OC_2H_5)_2(OCH_3)_3$	65.45	1258.23	32.08	-477.08
$C_{12}H_3Cl_2(OC_2H_5)_3(OCH_3)_2$	91.01	1347.30	16.59	-541.09
$C_{12}H_3Cl_2(OC_2H_5)_4(OCH_3)$	116.97	1434.80	1.01	-603.22
$C_{12}H_3Cl_2(OC_2H_5)(OCH_3)_4$	39.90	1169.26	47.56	-413.08
$C_{12}H_3Cl(OC_2H_5)(OCH_3)_5$	12.59	1288.12	62.01	-443.25
$C_{12}H_3Cl(OC_2H_5)_5(OCH_3)_1$	115.01	1643.37	0.03	-718.48
$C_{12}H_3Cl(OC_2H_5)_4(OCH_3)_2$	89.26	1555.14	15.56	-635.25
$C_{12}H_3Cl(OC_2H_5)_3(OCH_3)_3$	63.70	1466.16	31.05	-571.25
$C_{12}H_3Cl(OC_2H_5)_2(OCH_3)_4$	38.14	1377.09	46.53	-507.25
$C_{12}H_3(OC_2H_5)_2(OCH_3)_5$	10.84	1495.95	60.98	-537.42
$C_{12}H_3(OC_2H_5)(OCH_3)_6$	-39.41	1495.98	82.72	-586.55
$C_{12}H_3(OC_2H_5)_6(OCH_3)$	113.06	1851.94	-0.95	-793.42
$C_{12}H_3(OC_2H_5)_5(OCH_3)_2$	87.81	1761.87	14.46	-728.02
$C_{12}H_3(OC_2H_5)_4(OCH_3)_3$	61.95	1674.00	30.01	-665.42
$C_{12}H_3(OC_2H_5)_3(OCH_3)_4$	36.39	1585.02	45.50	-601.42
$C_{12}H_6Cl_2(OC_2H_5)OH$	84.70	789.92	-16.52	-328.97
$C_{12}H_5Cl_3(OC_2H_5)OH$	103.78	766.57	-14.46	-319.50
$C_{12}H_5Cl_2(OC_2H_5)_2OH$	102.03	974.30	-15.49	-413.67
$C_{12}H_4Cl_4(OC_2H_5)OH$	122.86	743.20	-12.41	-310.03
$C_{12}H_4Cl_3(OC_2H_5)_2OH$	137.23	892.73	-17.52	-330.33
$C_{12}H_4Cl_3(OC_2H_5)(OH)_2$	115.66	768.73	-12.51	-318.10
$C_{12}H_3Cl_4(OC_2H_5)(OH)_2$	134.74	745.27	-10.46	-308.68
$C_{12}H_5Cl_2(OC_2H_5)(OH)_2$	96.59	792.19	-14.57	-327.63
$C_{12}H_6Cl(OC_2H_5)(OH)_2$	77.51	815.65	-16.62	-337.10
$C_{12}H_6(OC_2H_5)(OH)_3$	70.32	841.38	-16.73	-345.23
$C_{12}H_6(OC_2H_5)_2(OH)_2$	85.50	988.36	-20.12	-386.62
$C_{12}H_6(OC_2H_5)_3(OH)$	117.83	1073.65	-12.39	-349.47

Compound	$C_p = a + b \cdot 10^{-3}\ T + c \cdot 10^{5}\ T^{-2} + d \cdot 10^{-6}\ T^{2}$ J mol^{-1} K^{-1}			
	a	b	c	d
$C_{12}H_5Cl(OC_2H_5)(OH)_3$	89.39	817.92	-14.67	-335.76
$C_{12}H_5(OC_2H_5)(OH)_4$	82.20	843.65	-14.77	-343.89
$C_{12}H_5(OC_2H_5)_2(OH)_3$	95.45	997.62	-17.68	-394.16
$C_{12}H_5(OC_2H_5)_3(OH)_2$	145.12	1020.39	-29.81	-277.54
$C_{12}H_5(OC_2H_5)_4(OH)$	144.59	1224.01	-29.23	-390.92
$C_{12}H_4Cl_2(OC_2H_5)(OH)_3$	108.47	794.46	-12.61	-326.29
$C_{12}H_4Cl(OC_2H_5)(OH)_4$	101.28	820.19	-12.72	-334.42
$C_{12}H_4(OC_2H_5)(OH)_5$	94.09	845.92	-12.82	-342.55
$C_{12}H_4(OC_2H_5)_2(OH)_4$	99.53	1028.02	-13.75	-428.58
$C_{12}H_4(OC_2H_5)_3(OH)_3$	104.97	1210.23	-14.68	-514.62
$C_{12}H_4(OC_2H_5)_4(OH)_2$	110.41	1392.33	-15.60	-600.66
$C_{12}H_4(OC_2H_5)_5(OH)$	115.85	1574.44	-16.53	-1015.73
$C_{12}H_4Cl_2(OC_2H_5)_2(OH)_2$	113.91	976.57	-13.54	-412.32
$C_{12}H_4Cl_2(OC_2H_5)_3(OH)$	119.35	1158.77	-14.47	-498.36
$C_{12}H_4Cl(OC_2H_5)_2(OH)_3$	106.72	1002.30	-13.64	-420.45
$C_{12}H_4Cl(OC_2H_5)_3(OH)_2$	130.12	1119.77	-19.12	-424.21
$C_{12}H_4Cl(OC_2H_5)_4(OH)$	117.60	1366.61	-15.50	-592.53
$C_{12}H_5Cl(OC_2H_5)_2(OH)_2$	94.83	1000.03	-15.60	-421.80
$C_{12}H_5Cl(OC_2H_5)_3(OH)$	100.27	1182.23	-16.52	-507.83
$C_{12}H_3Cl_4(OC_2H_5)_2(OH)$	140.18	927.38	-11.38	-394.72
$C_{12}H_3C_{l3}(OC_2H_5)_3(OH)$	138.43	1135.31	-12.41	-488.89
$C_{12}H_3Cl_3(OC_2H_5)_2(OH)_2$	132.99	953.11	-11.49	-402.85
$C_{12}H_3Cl_3(OC_2H_5)(OH)_3$	105.31	851.18	-4.92	-418.73
$C_{12}H_3Cl_2(OC_2H_5)_2(OH)_3$	125.80	978.84	-11.59	-410.98
$C_{12}H_3Cl_2(OC_2H_5)_3(OH)_2$	131.24	1161.04	-12.52	-497.02
$C_{12}H_3Cl_2(OC_2H_5)_4(OH)$	137.09	1341.67	-13.55	-581.18
$C_{12}H_3Cl_2(OC_2H_5)(OH)_4$	120.36	796.73	-10.66	-324.94
$C_{12}H_3Cl(OC_2H_5)(OH)_5$	113.17	822.46	-10.77	-333.07
$C_{12}H_3Cl(OC_2H_5)_5(OH)$	135.13	1550.24	-14.53	-696.44
$C_{12}H_3Cl(OC_2H_5)_4(OH)_2$	129.49	1368.87	-13.55	-591.18
$C_{12}H_3Cl(OC_2H_5)_3(OH)_3$	124.05	1186.77	-12.62	-505.15
$C_{12}H_3Cl(OC_2H_5)_2(OH)_4$	118.61	1004.56	-11.69	-419.11
$C_{12}H_3(OC_2H_5)_2(OH)_5$	111.41	1030.29	-11.80	-427.24
$C_{12}H_3(OC_2H_5)(OH)_6$	81.28	937.19	-4.61	-454.34
$C_{12}H_3(OC_2H_5)_6(OH)$	133.17	1758.81	-15.50	-771.39
$C_{12}H_3(OC_2H_5)_5(OH)_2$	128.04	1575.60	-14.65	-683.95
$C_{12}H_3(OC_2H_5)_4(OH)_3$	122.29	1394.60	-13.65	-599.31
$C_{12}H_3(OC_2H_5)_3(OH)_4$	116.85	1212.50	-12.72	-513.28

Conclusions

Thermochemical parameters, such as standard enthalpy of formation, enthalpy increment from 0 to 298 K, standard heat capacity and its temperature dependence, and entropy, were calculated for the ethoxy-, ethoxymethoxy- ethoxyhydroxy- derivatives (125 substances) formed from polychlorinated biphenyls congeners by chemical interaction with sodium methoxide in dimethyl sulfoxide and ethanol.

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